

Multicomponent, Hydrogen-Bonded Cylindrical Capsules

Supporting Information

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General procedure for encapsulation of gaseous guest in 1.2₄.1:

A 1 mM solution of capsule **1.2₄.1** was formed by addition of **1** (4 mg, 0.0024 mmol) and **2c** (3 mg, 0.0055 mmol) in Mesitylene-*d*₁₂ (0.6 mL) to a 5-mm NMR. The gas was bubbled into the solution slowly to avoid excess foaming for 10 s. The tube was placed in an ultrasonic bath (230 W) and sonicated for 5-10 min.

General procedure for encapsulation of gaseous guest in 1.2₄.1:

A 1 mM solution of capsule **1.2.4.1** was formed by addition of **1** (4 mg, 0.0024 mmol) and **2c** (3 mg, 0.0055 mmol) in Mesitylene-*d*₁₂ (0.6 mL) to a 5-mm NMR. The neat guest (5 µL or 1mg) was added into the solution and the tube was placed in an ultrasonic bath (230W) and sonicated for 5-10 min.

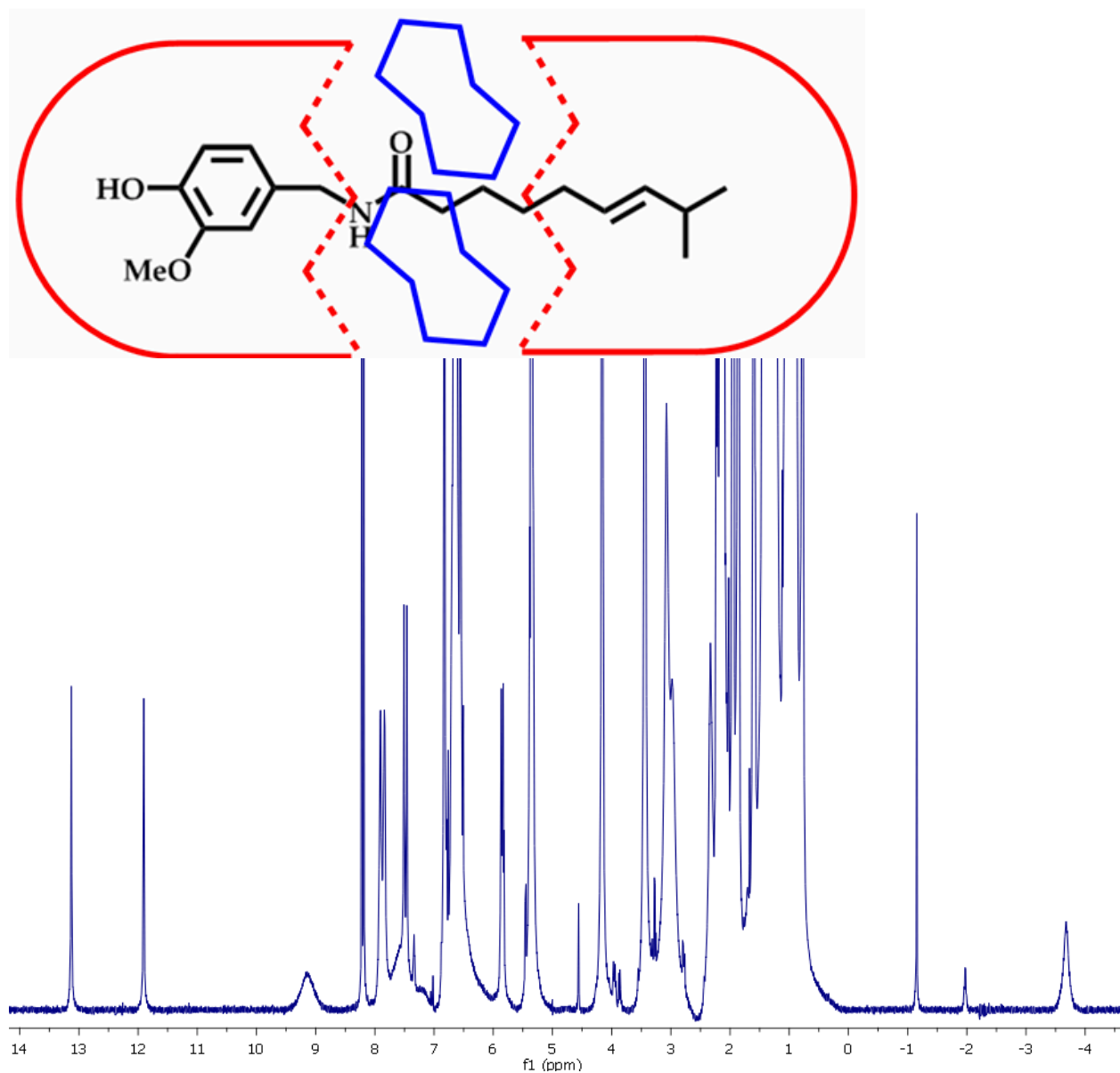
Procedure for coencapsulation of Xenon with Alkanes in 1.2.4.1:

A 1 mM solution of capsule **1.2.4.1** was formed by addition of **1** (4 mg, 0.0024 mmol) and **2c** (3 mg, 0.0055 mmol) in Mesitylene-*d*₁₂ (0.6 mL) to a 5-mm NMR. The neat alkane (5 µL or 1mg) was added into the solution and Xenon gas was bubbled into the solution briefly (5 s) and the tube was placed in an ultrasonic bath (230W) and sonicated for 5-10 min.

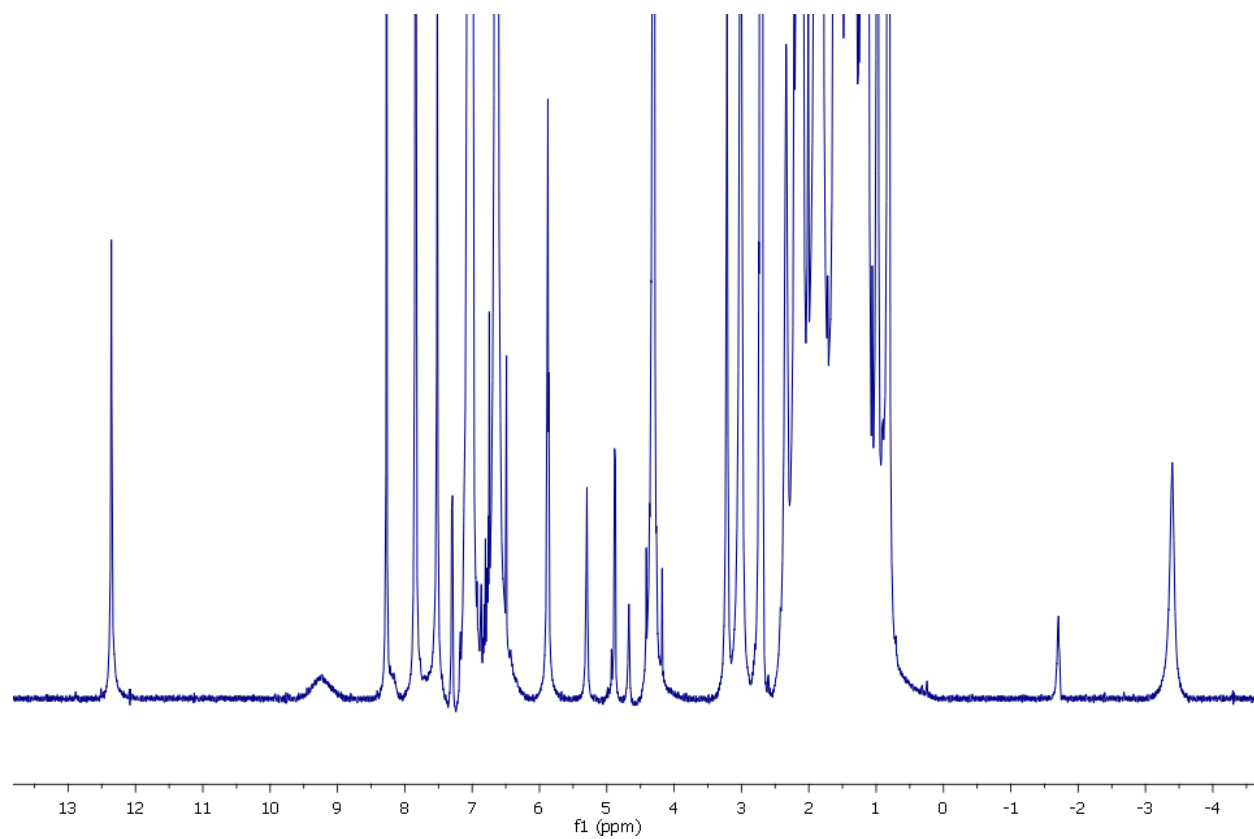
Reference 32:

Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

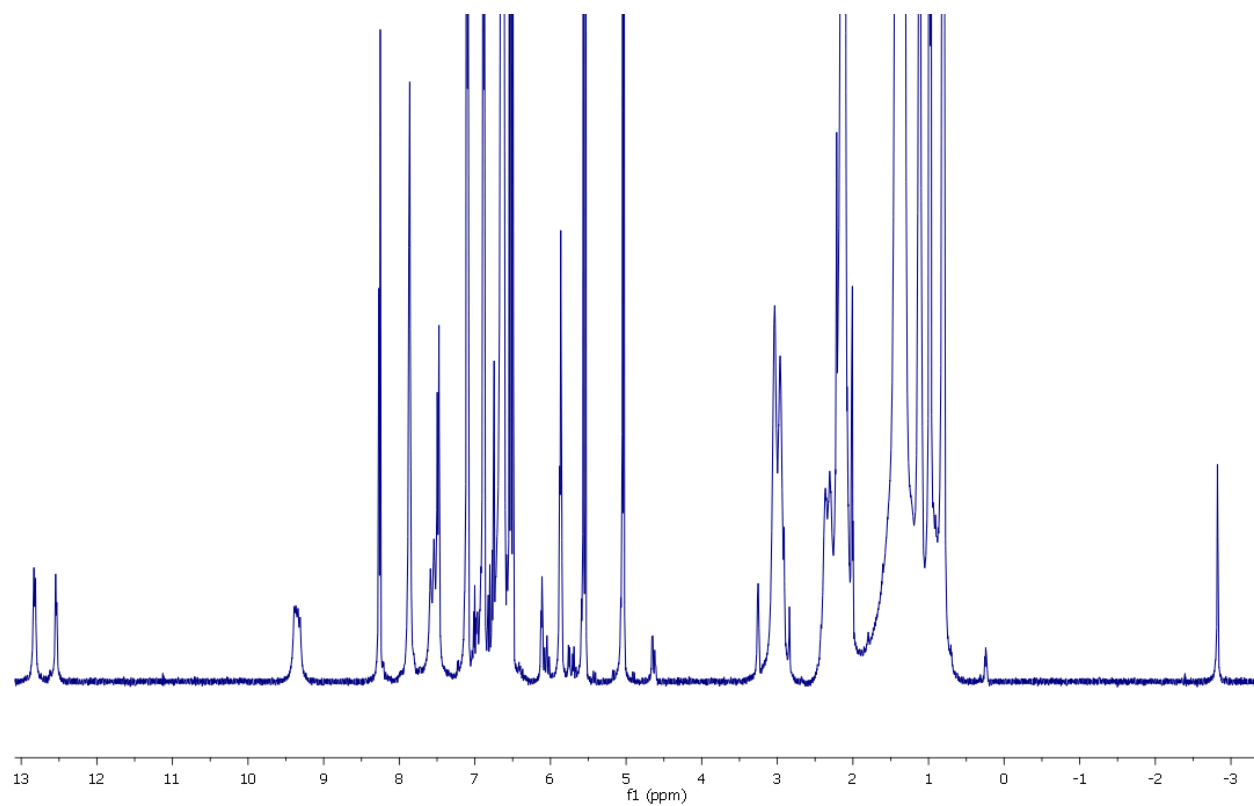
¹H NMR spectra of encapsulated Capsaicin in 1.2.4.1 :



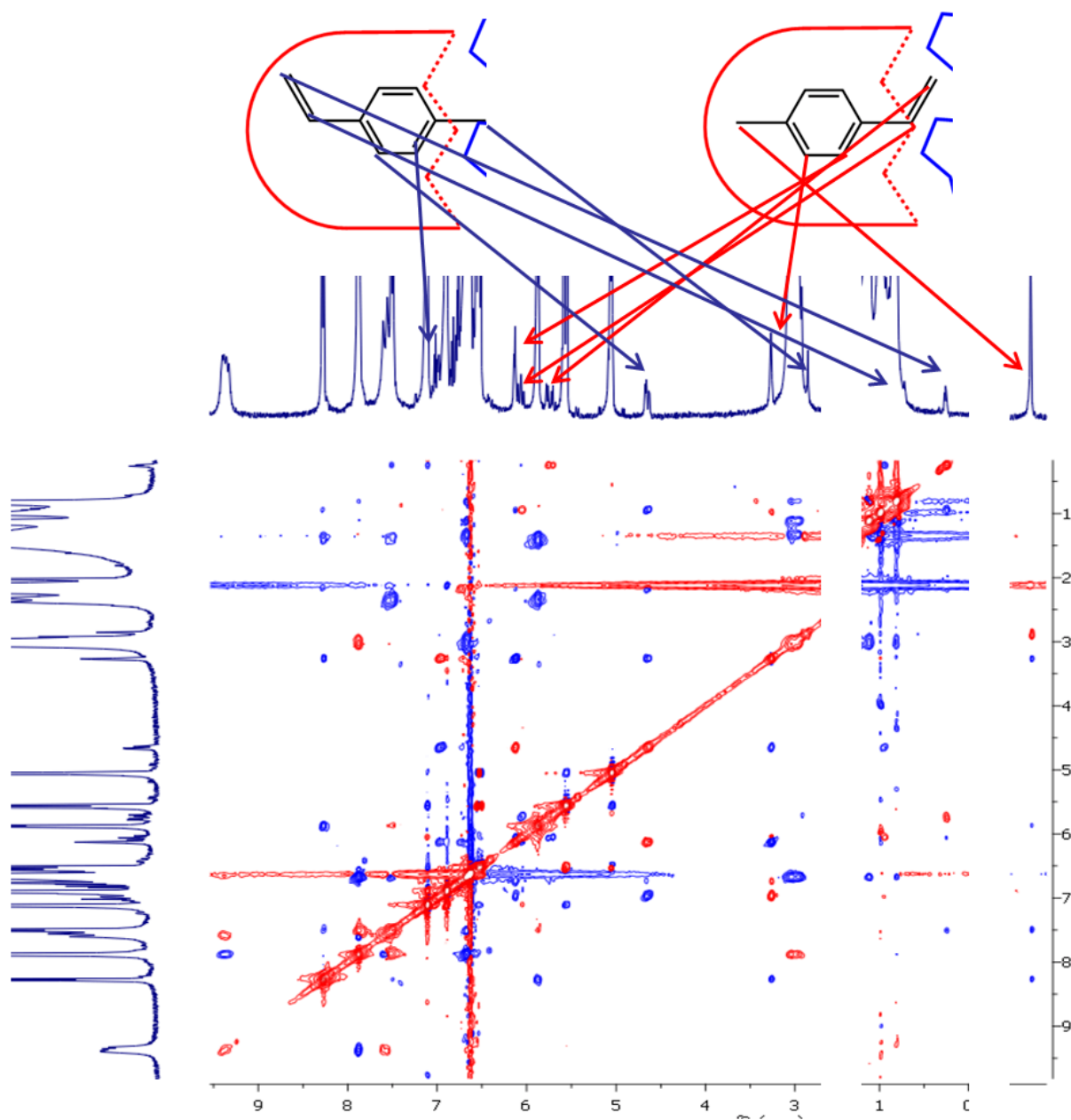
^1H NMR spectra of encapsulated *p*-isopropyl benzyl alcohol in 1.2.1 :



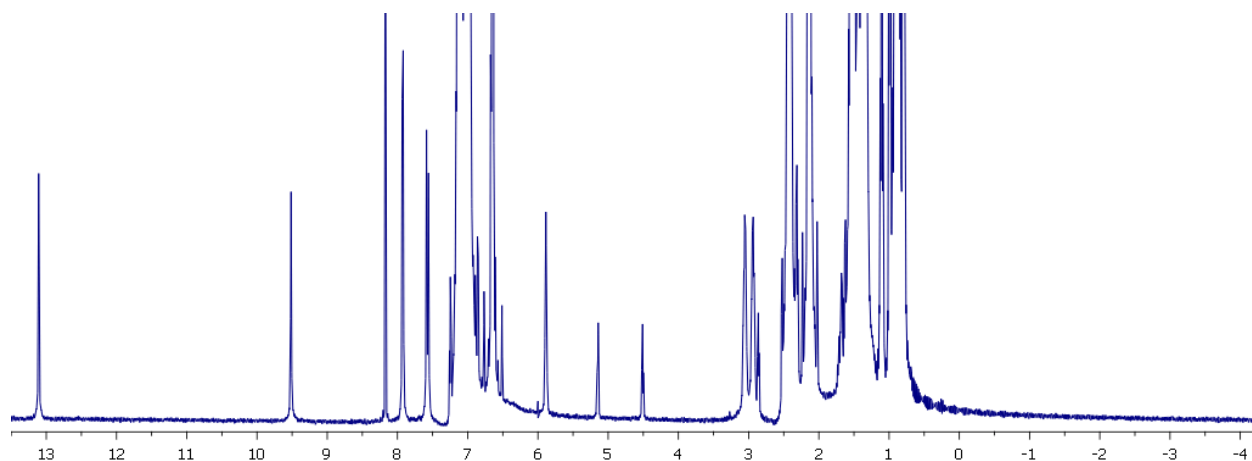
^1H NMR spectra of encapsulated *p*-methyl styrene in 1.2₄.1 :



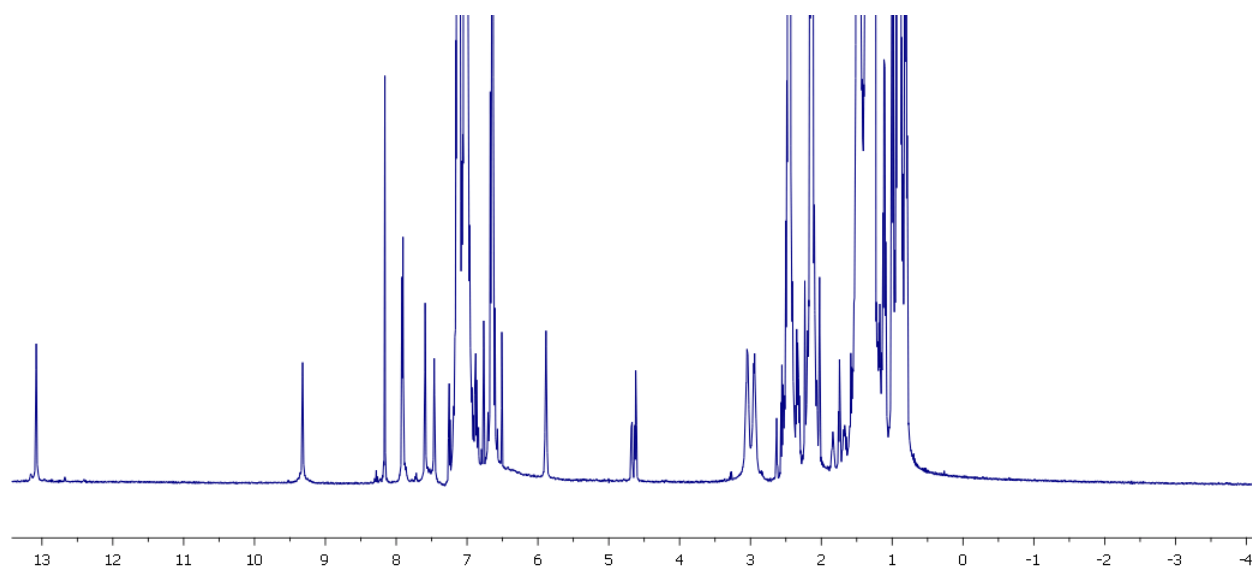
2D ROSEY spectra of encapsulated *p*-methyl styrene in 1.2₄.1:



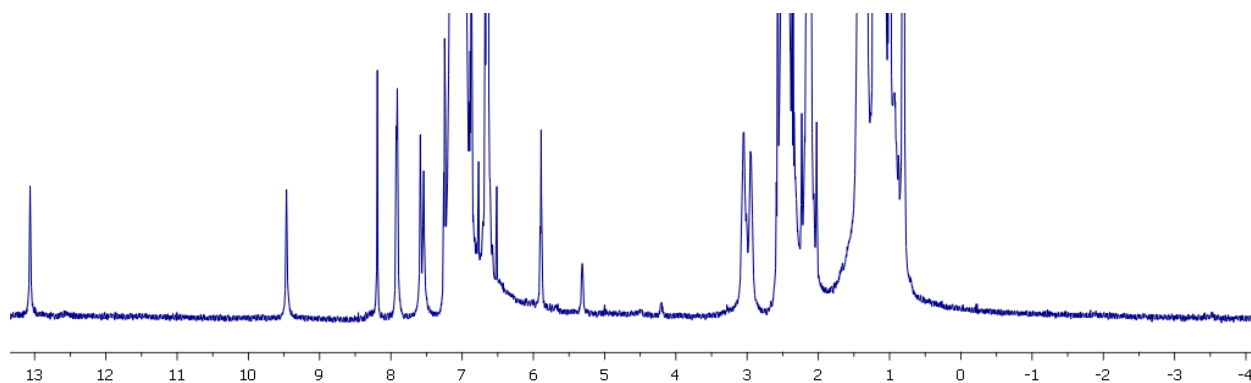
^1H NMR spectra of encapsulated n-propyl benzene in 1.2₄.1



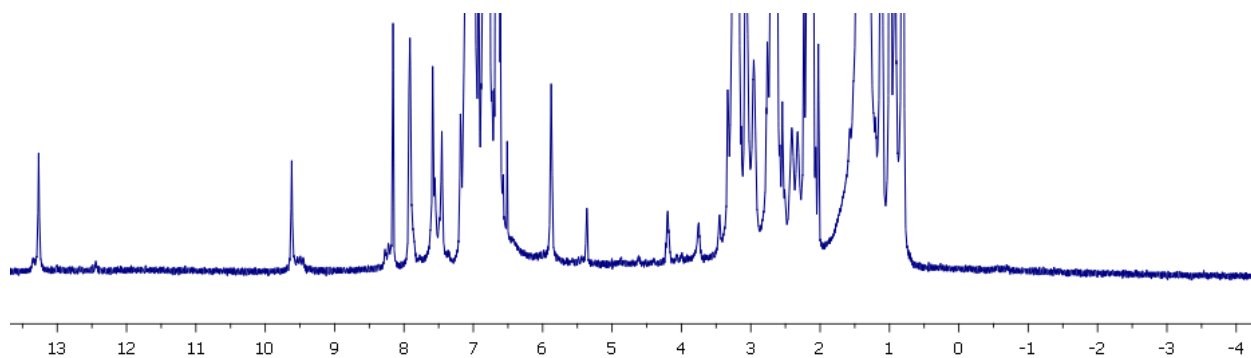
^1H NMR spectra of encapsulated n-butyl benzene in 1.2₄.1



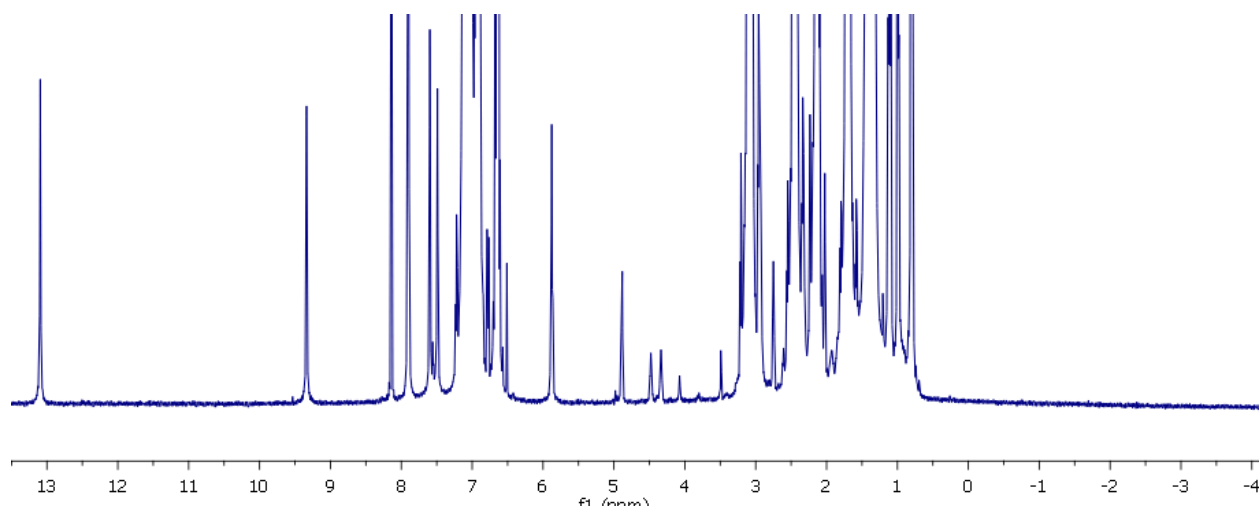
^1H NMR spectra of encapsulated n-ethyl benzene in 1.2₄.1



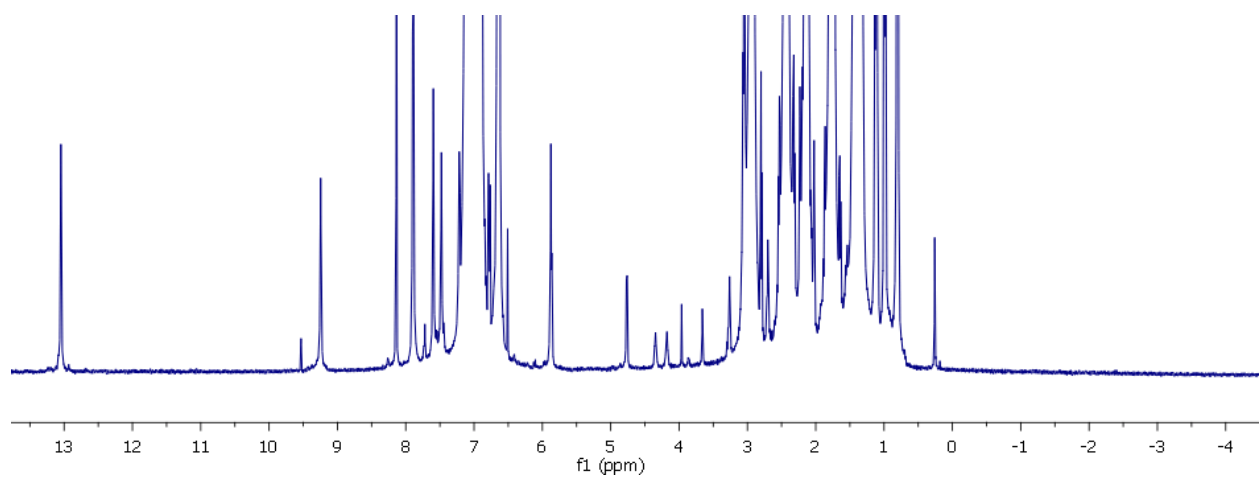
^1H NMR spectra of encapsulated (2-chloroethyl)benzene in 1.2₄.1



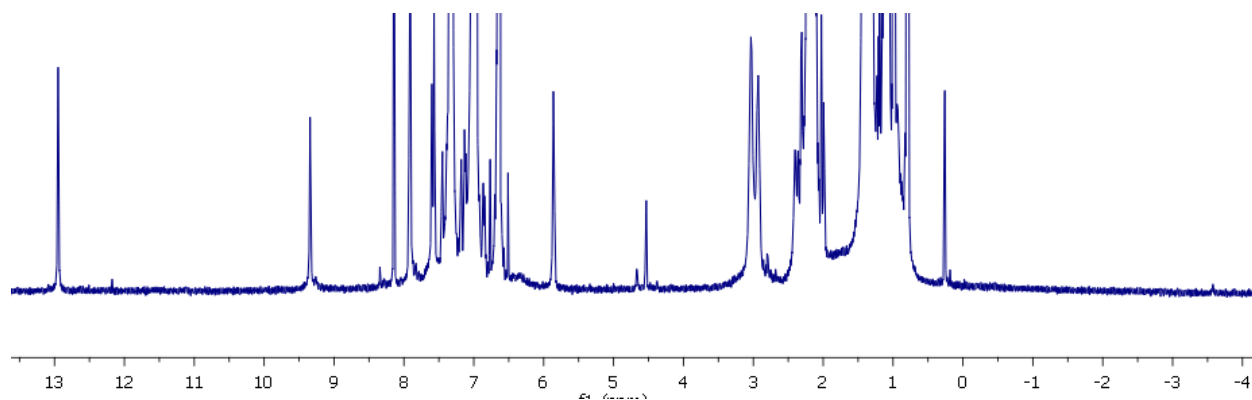
^1H NMR spectra of encapsulated (3-chloropropyl)benzene in 1.2₄.1



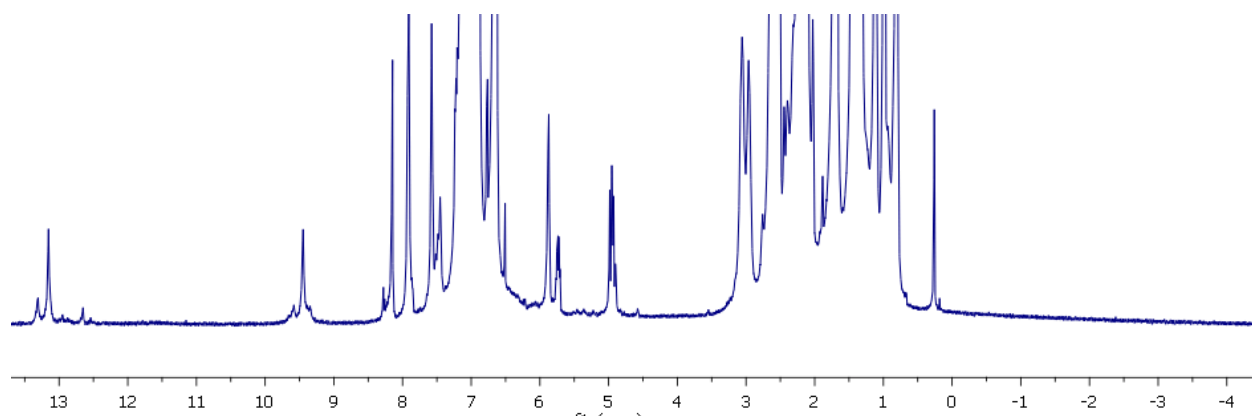
^1H NMR spectra of encapsulated (3-bromopropyl)benzene in 1.2₄.1



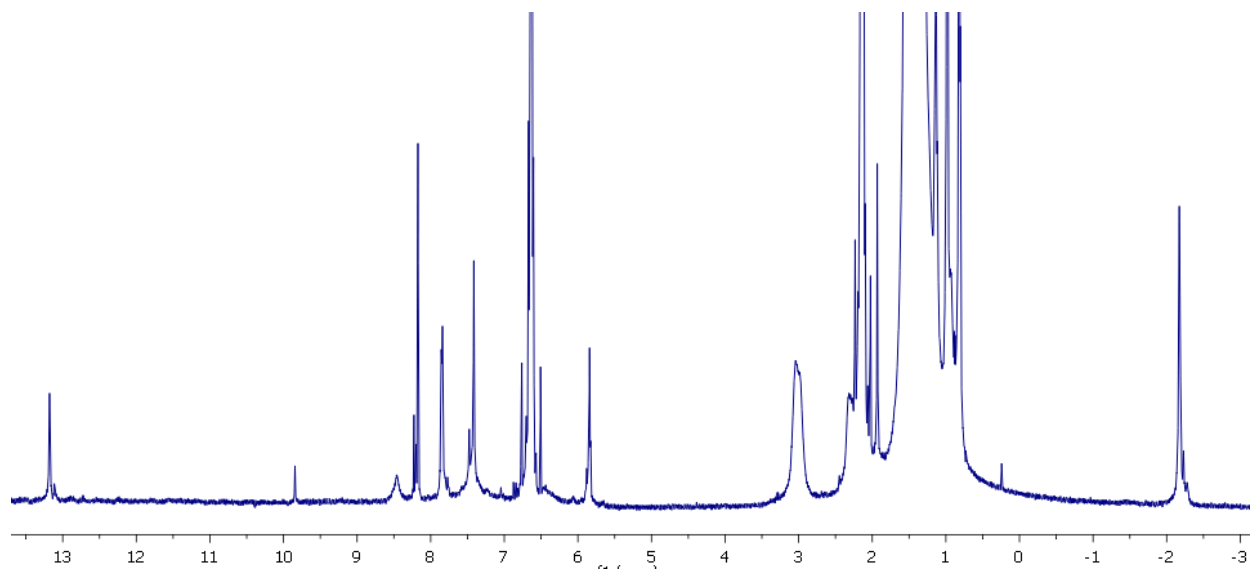
^1H NMR spectra of encapsulated 1-phenyl-1-butyne in 1.2₄.1



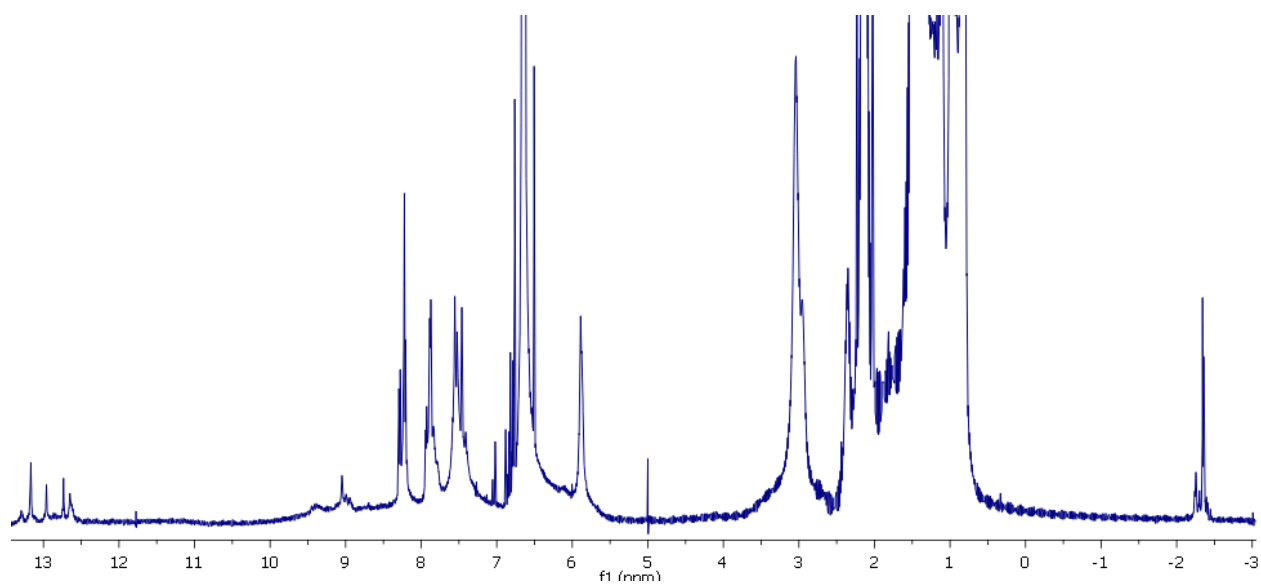
^1H NMR spectra of encapsulated 4-phenyl-1-butyne in 1.2₄.1



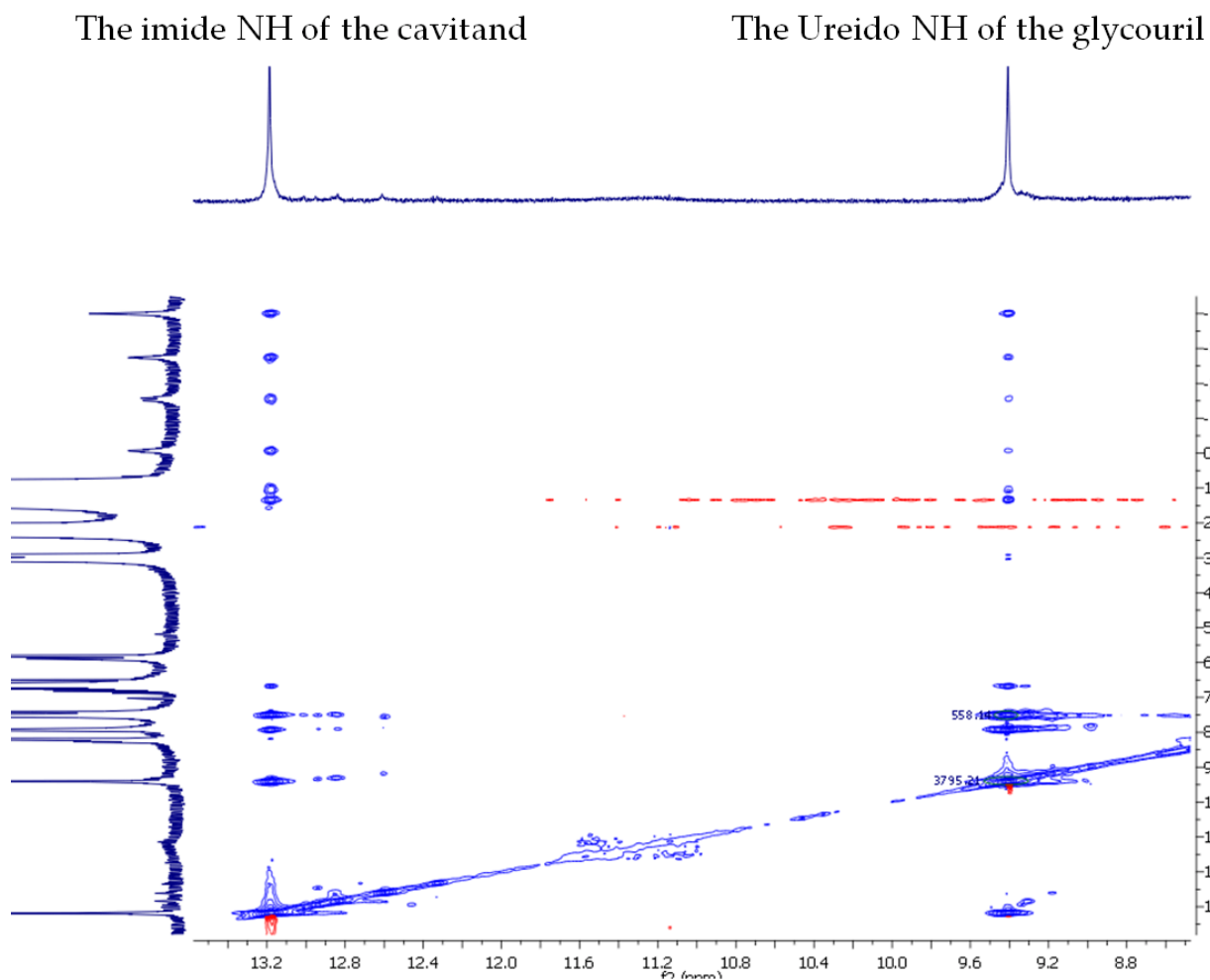
^1H NMR Assignment of encapsulated Cyclohexane in 1.2₄.1



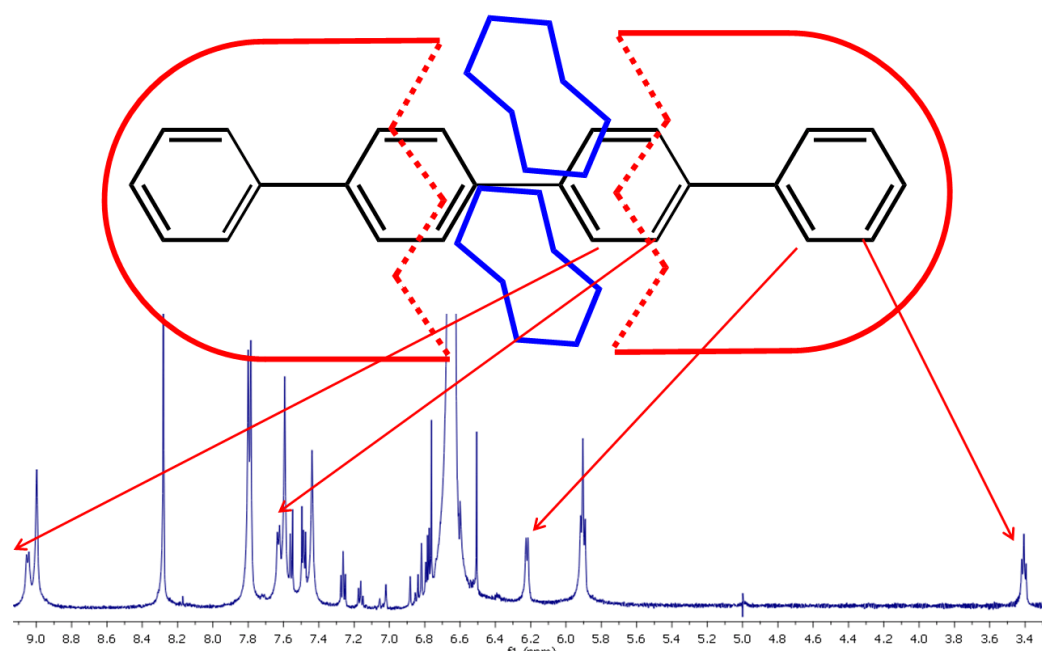
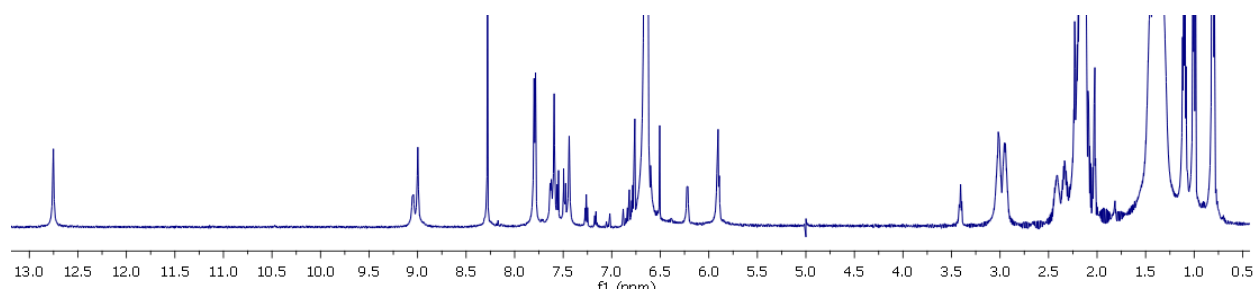
^1H NMR Assignment of encapsulated Cyclopentane in 1.2₄.1



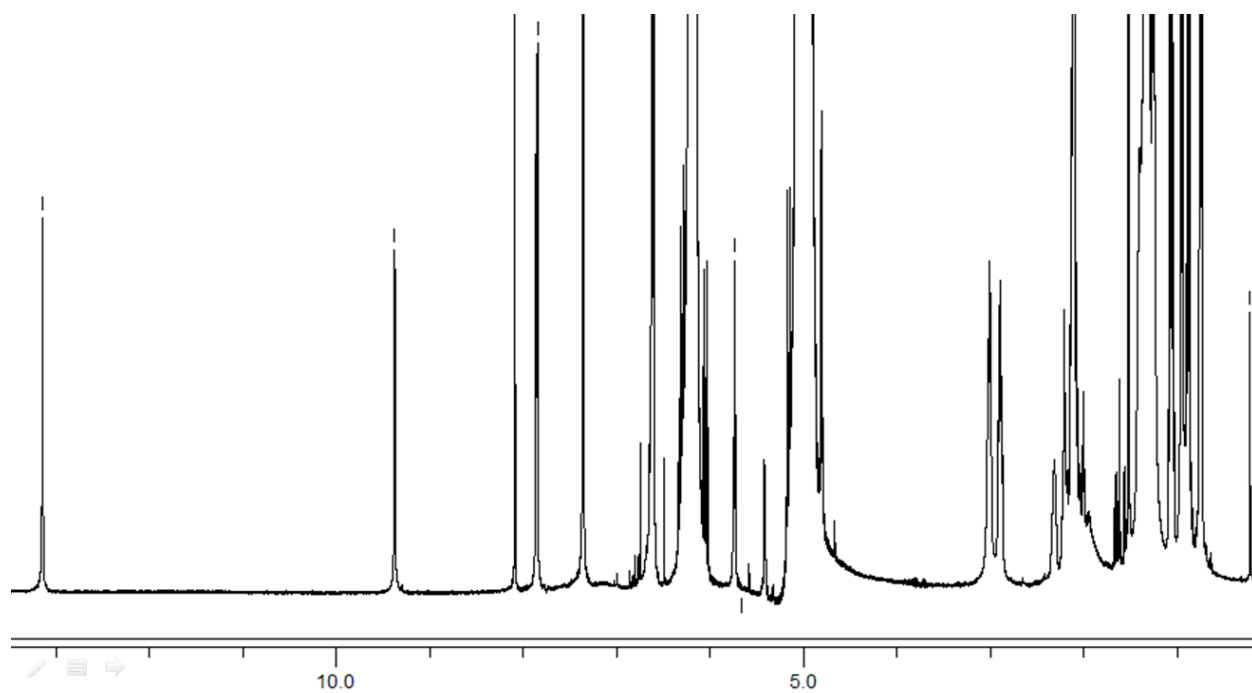
2D NOESY spectra of encapsulated *n*-hexane in 1.2₄.1:



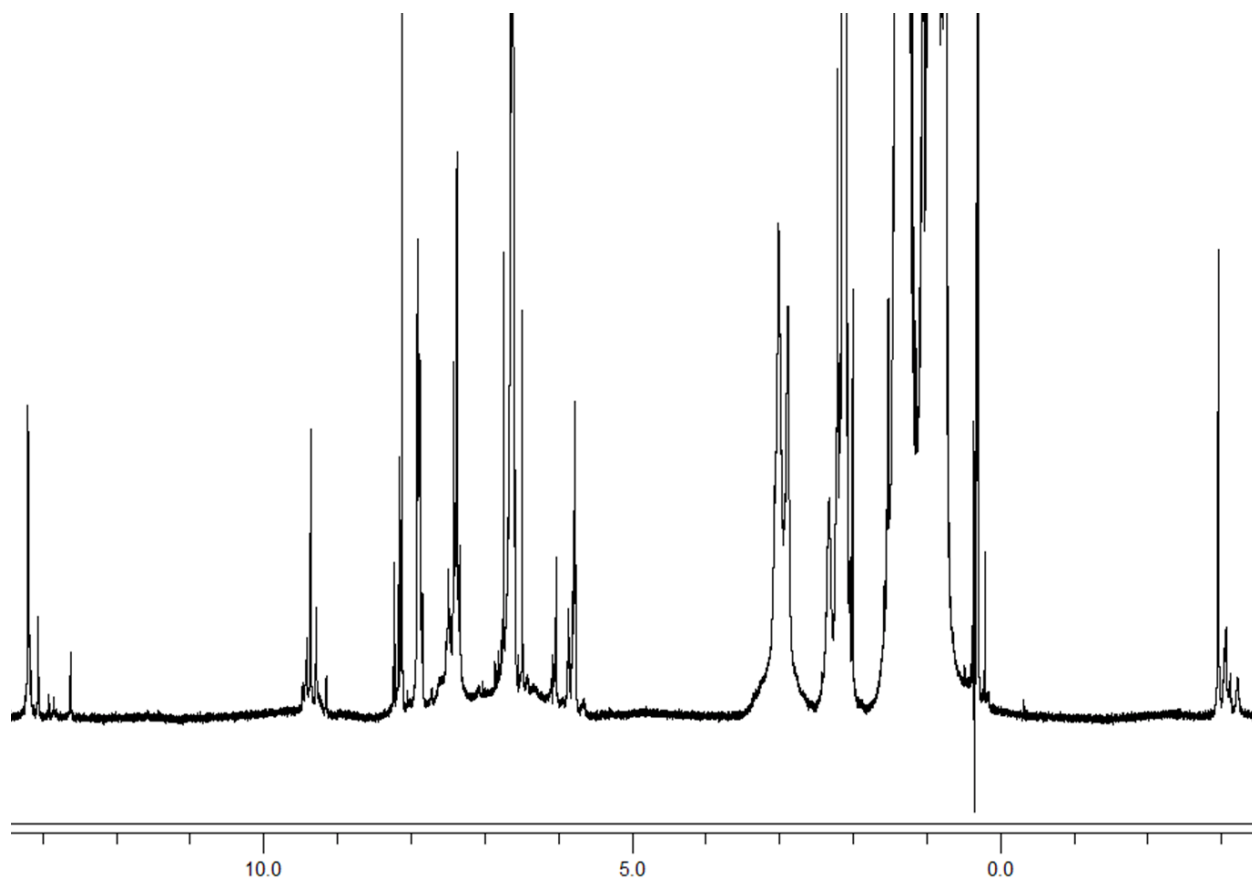
^1H NMR Assignment of encapsulated *p*-quaterphenyl in 1.2₄.1



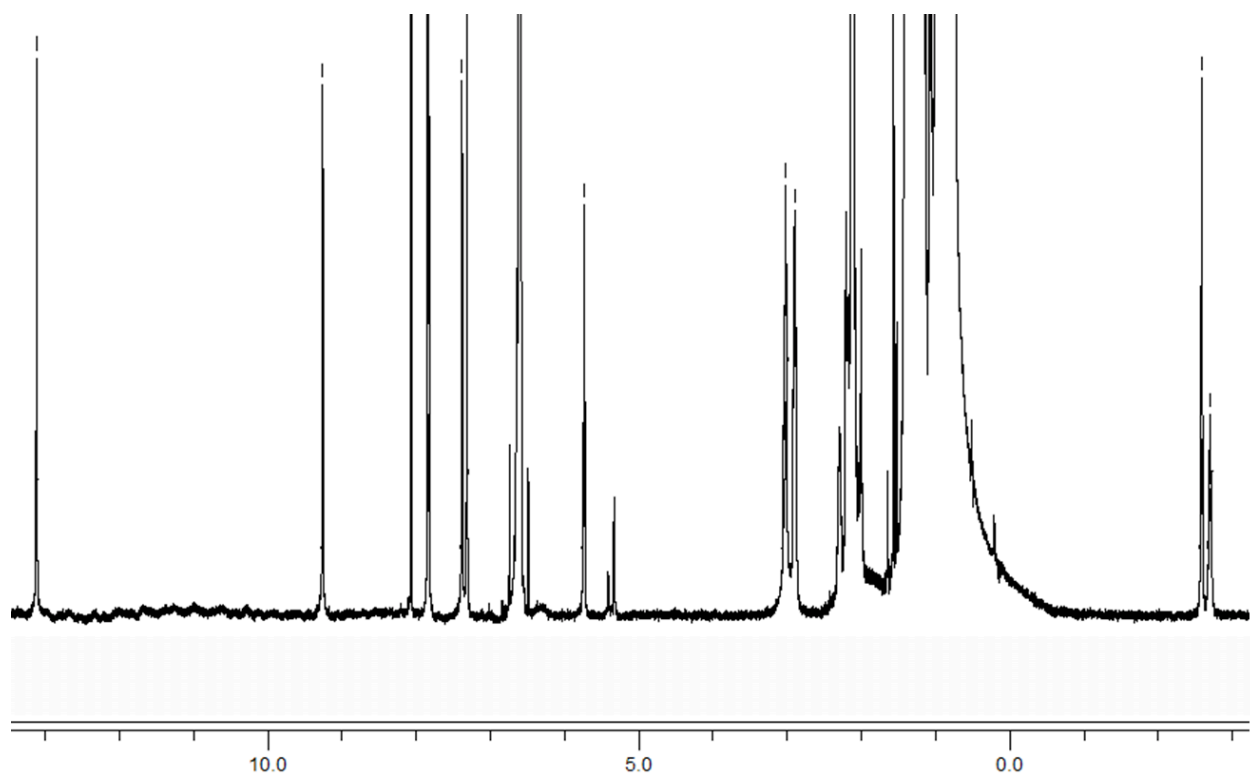
¹H NMR spectra of encapsulated 1,3-butadiene in 1.2₄.1 :



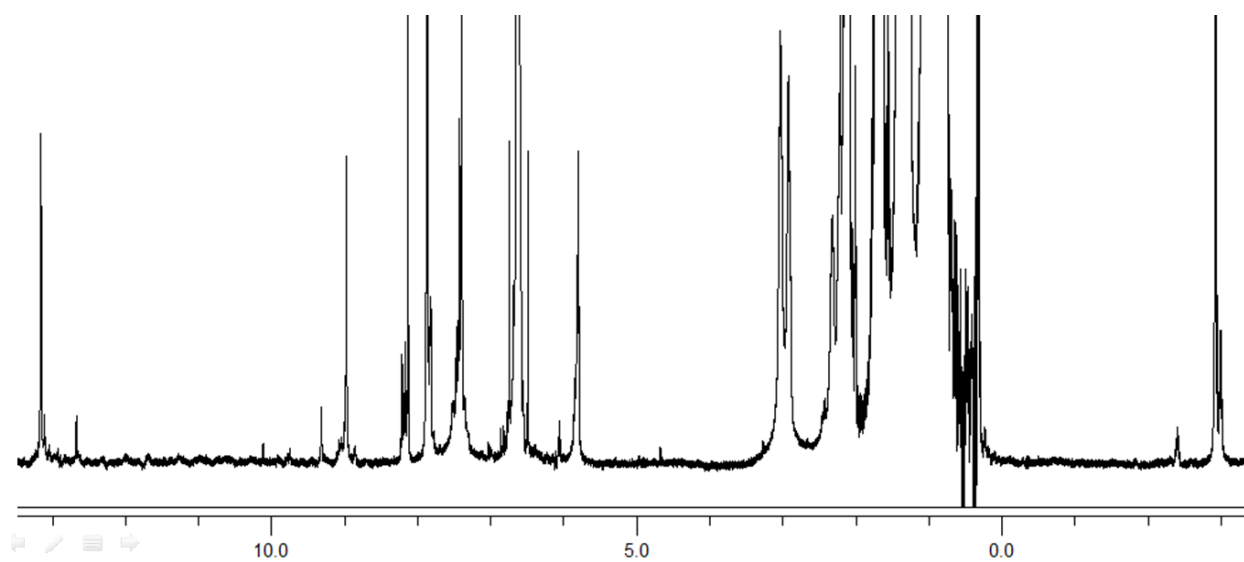
^1H NMR spectra of encapsulated propane in 1.2₄.1 :



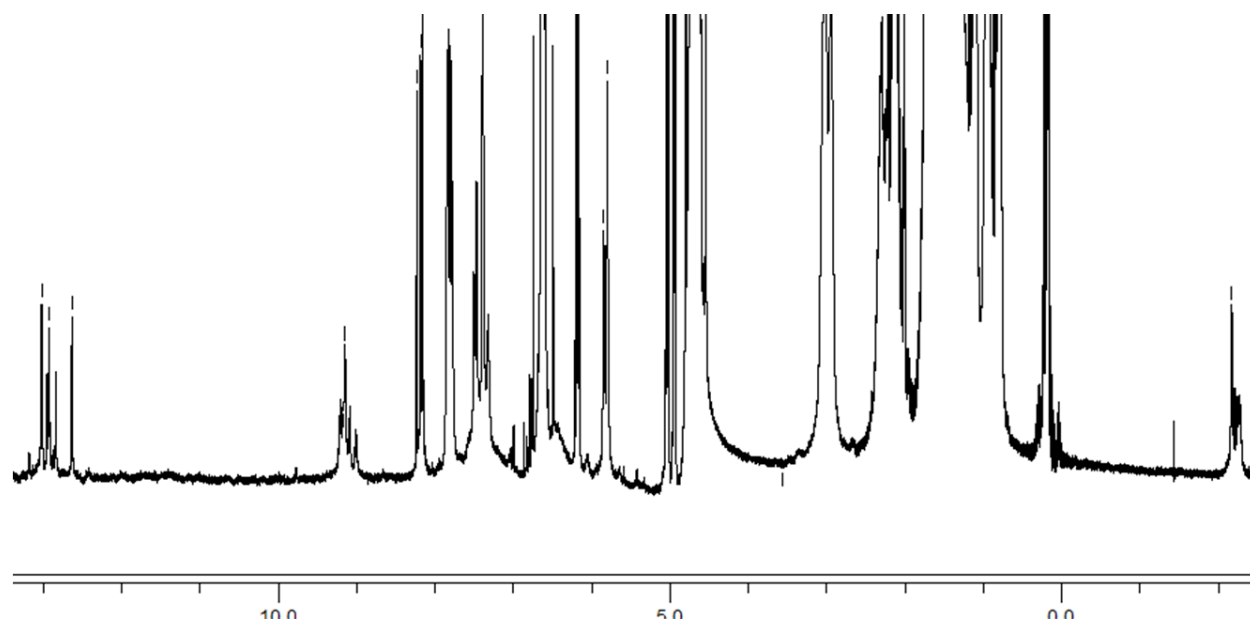
^1H NMR spectra of encapsulated butane in 1.2₄.1 :



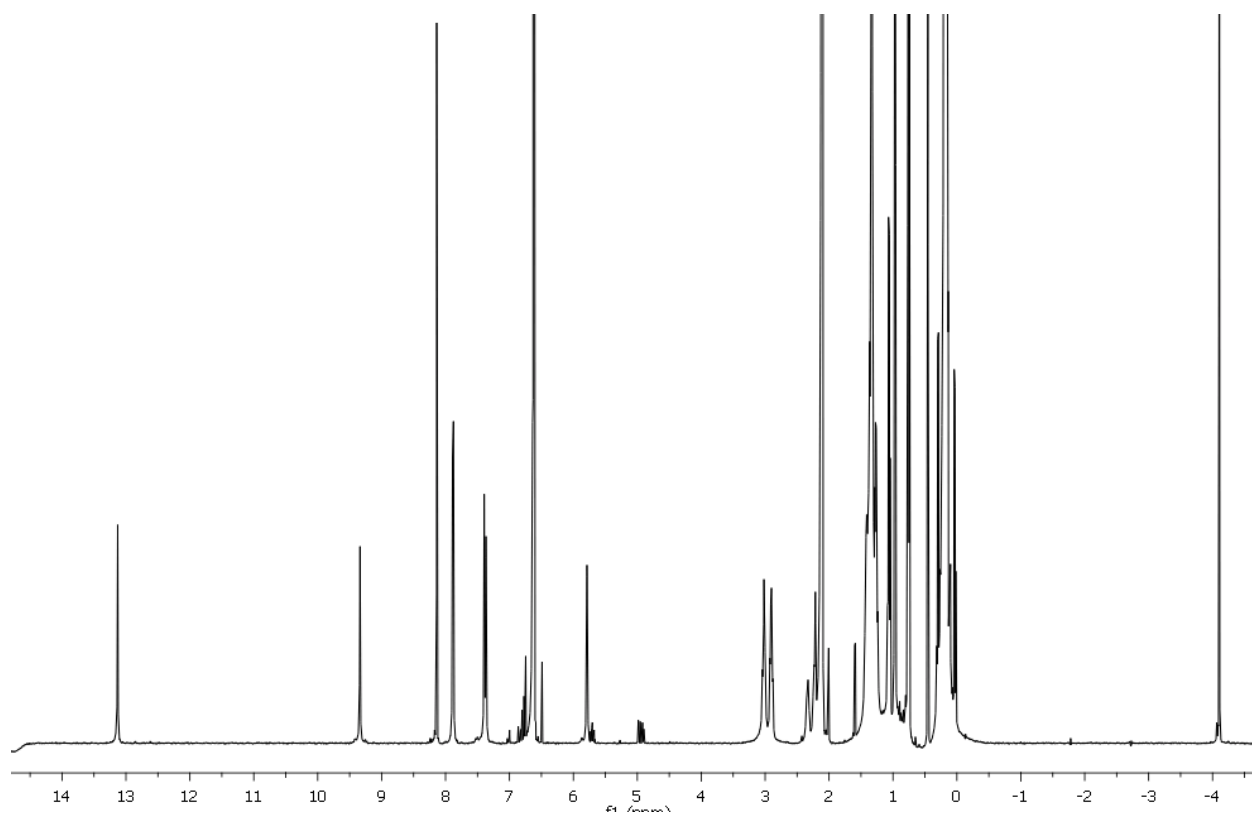
^1H NMR spectra of encapsulated isobutane in 1.2₄.1 :



^1H NMR spectra of encapsulated 2-methylpropene in 1.2₄.1 :



^1H NMR spectra of encapsulated Cyclopropane in 1.2₄.1 :



2D ROSEY spectra of coencapsulation of propane and nonane in 1.2₄.1:

